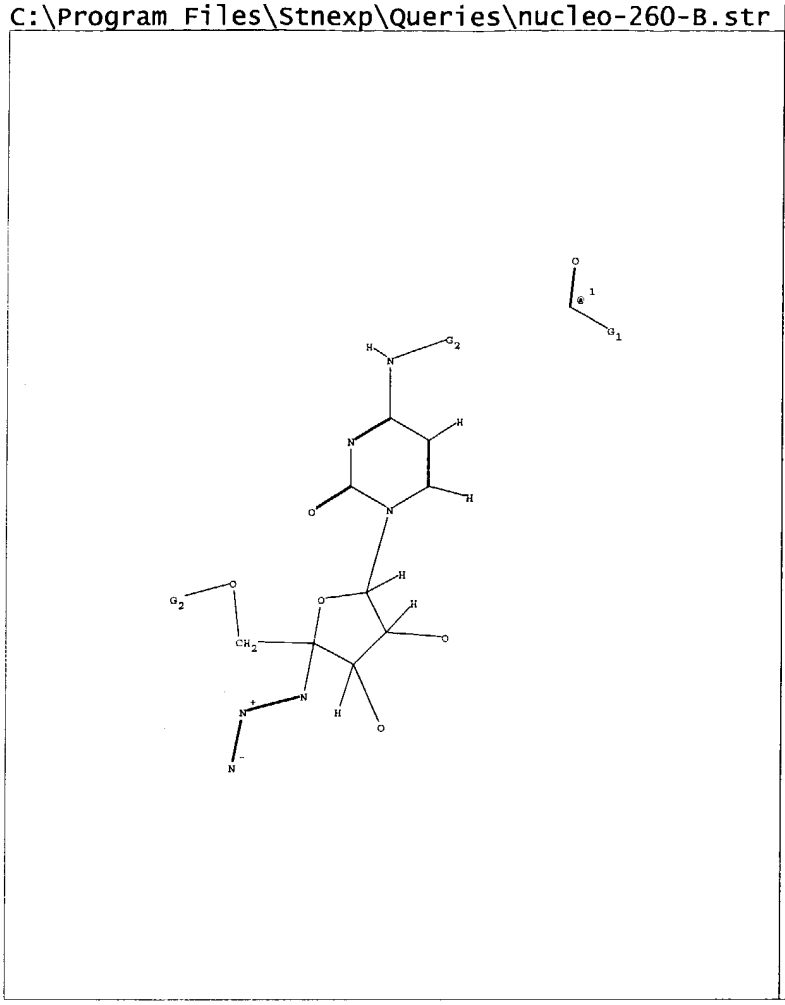
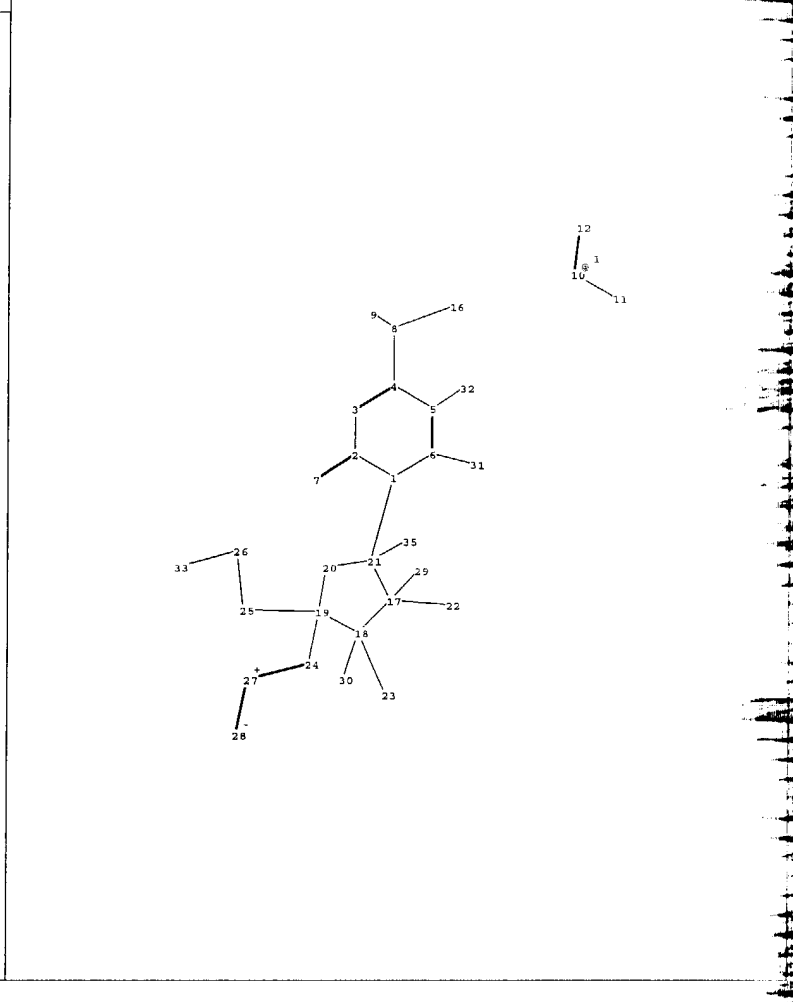
C:\Program Files\Stnexp\Queries\nucleo-260-B.str





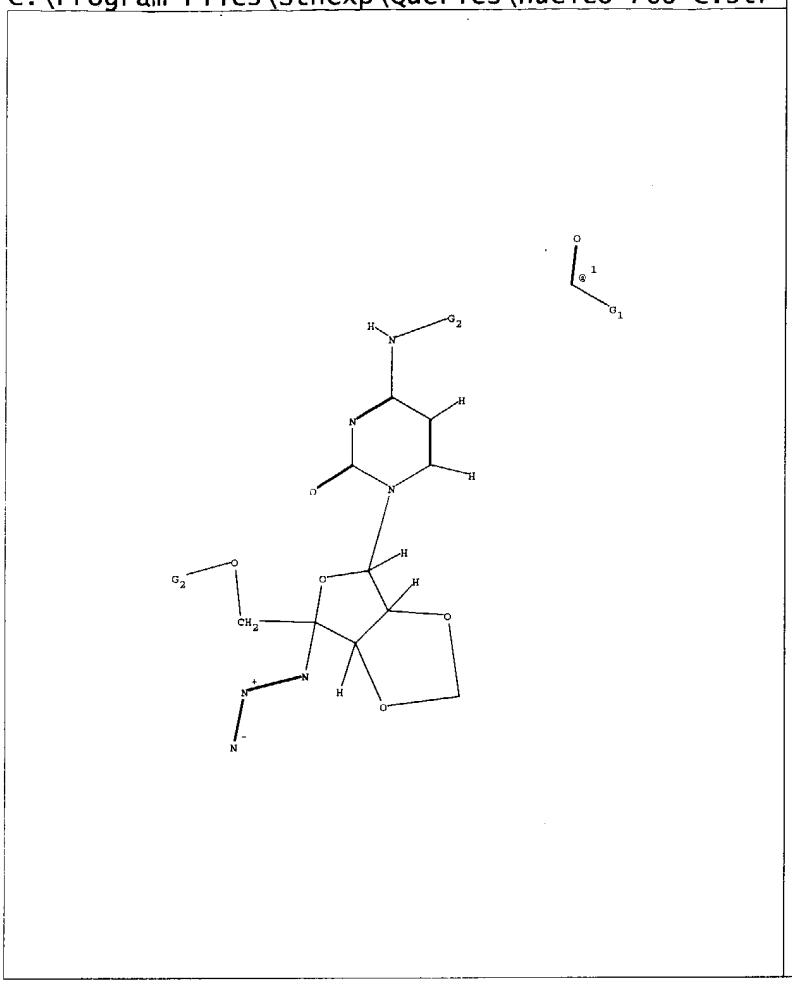
chain nodes :
7 8 9 10 11 12 16 22 23 24 25 26 27 28 29 30 31 32 33 35
ring nodes :
1 2 3 4 5 6 17 18 19 20 21
chain bonds :
1-21 2-7 4-8 5-32 6-31 8-9 8-16 10-12 10-11 17-22 17-29 18-23 18-30 19-24
19-25 21-35 24-27 25-26 26-33 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-21 18-19 19-20 20-21
exact/norm bonds :
1-2 1-6 1-21 2-3 2-7 3-4 4-5 4-8 5-6 8-16 10-12 10-11 17-18 17-21 17-22
18-19 18-23 19-20 19-24 20-21 24-27 26-33 27-28
exact bonds :
5-32 6-31 8-9 17-29 18-30 19-25 21-35 25-26

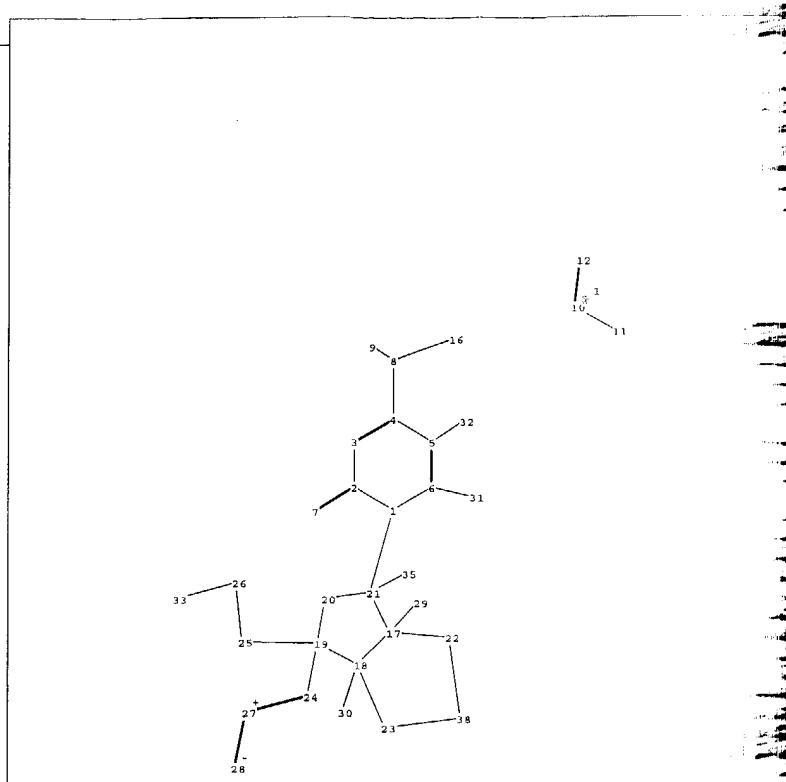
G1:O,S,N,C

G2:H,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS

C:\Program Files\Stnexp\Queries\nucleo-760-C.str





chain nodes :
7 8 9 10 11 12 16 24 25 26 27 28 29 30 31 32 33 35
ring nodes :
1 2 3 4 5 6 17 18 19 20 21 22 23 38
chain bonds :
1-21 2-7 4-8 5-32 6-31 8-9 8-16 10-12 10-11 17-29 18-30 19-24 19-25 21-35
24-27 25-26 26-33 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-21 17-22 18-19 18-23 19-20 20-21 22-38 23-38
exact/norm bonds :
1-2 1-6 1-21 2-3 2-7 3-4 4-5 4-8 5-6 8-16 10-12 10-11 17-18 17-21 17-22
18-19 18-23 19-20 19-24 20-21 22-38 23-38 24-27 26-33 27-28
exact bonds :
5-32 6-31 8-9 17-29 18-30 19-25 21-35 25-26

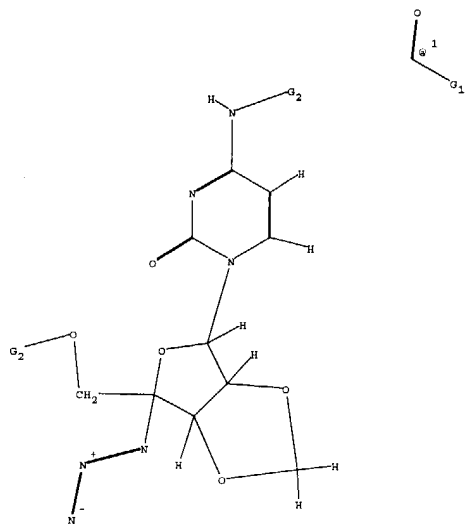
G1:O,S,N,C

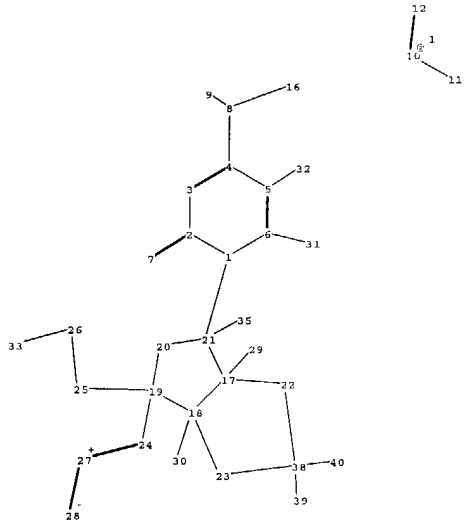
G2:H,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS 38:Atom

```
=> d his

     (FILE 'HOME' ENTERED AT 18:00:44 ON 10 AUG 2004)

     FILE 'REGISTRY' ENTERED AT 18:00:56 ON 10 AUG 2004
L1                STRUCTURE UPLOADED
L2              1 S L1 SSS SAM
L3              8 S L1 SSS FULL

     FILE 'CAPLUS, MEDLINE' ENTERED AT 18:02:57 ON 10 AUG 2004
L4              1 S L3
```

C:\Program Files\Stnexp\Queries\nucleo-760-D.str





chain nodes :
7 8 9 10 11 12 16 24 25 26 27 28 29 30 31 32 33 35 39 40
ring nodes :
1 2 3 4 5 6 17 18 19 20 21 22 23 38
chain bonds :
1-21 2-7 4-8 5-32 6-31 8-9 8-16 10-12 10-11 17-29 18-30 19-24 19-25 21-35
24-27 25-26 26-33 27-28 38-39 38-40
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-21 17-22 18-19 18-23 19-20 20-21 22-38 23-38
exact/norm bonds :
1-2 1-6 1-21 2-3 2-7 3-4 4-5 4-8 5-6 8-16 10-12 10-11 17-18 17-21 17-22
18-19 18-23 19-20 19-24 20-21 22-38 23-38 24-27 26-33 27-28
exact bonds :
5-32 6-31 8-9 17-29 18-30 19-25 21-35 25-26 38-39 38-40

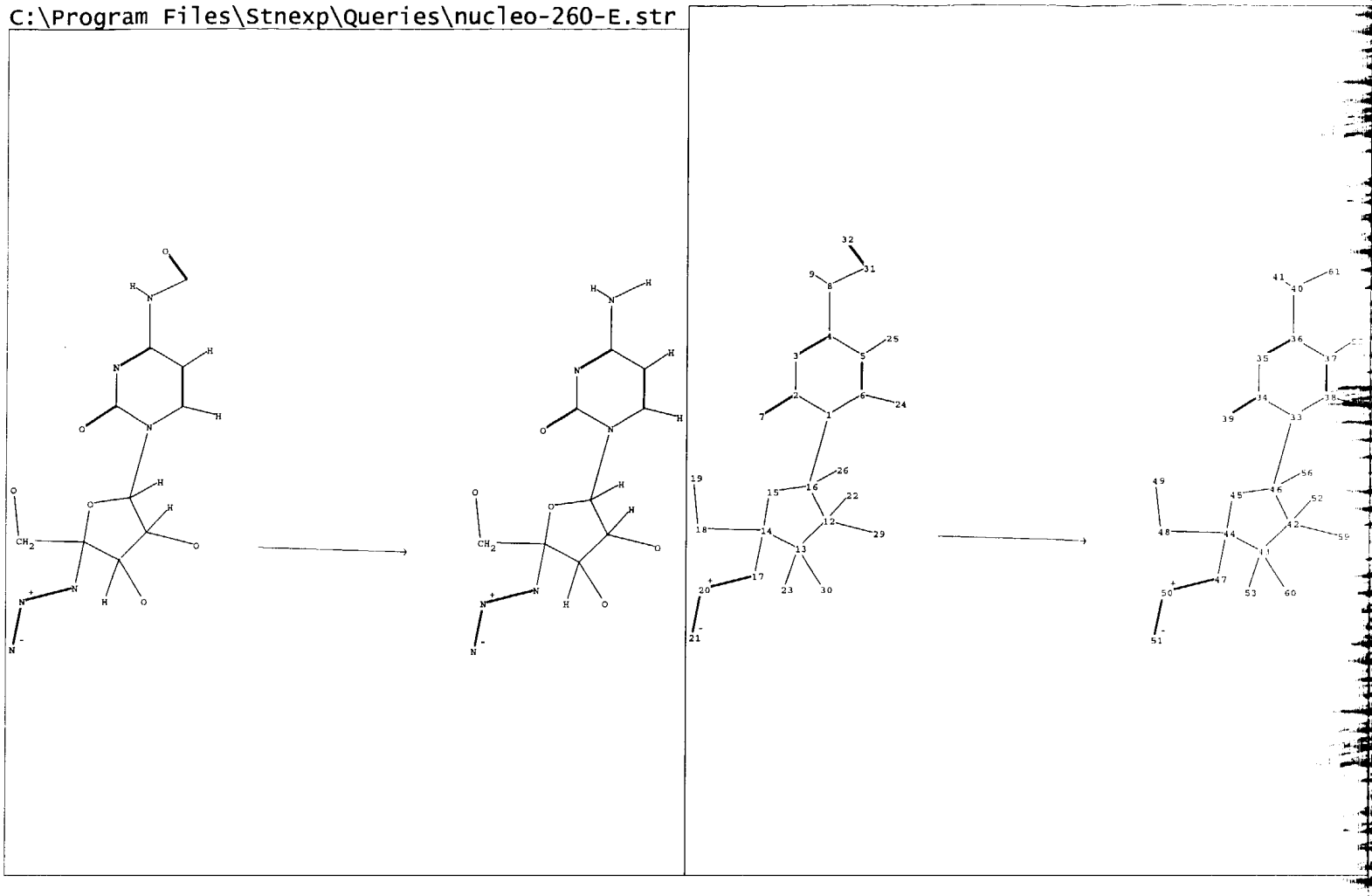
G1:O,S,N,C

G2:H,[*1]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 35:CLASS 38:Atom 39:CLASS 40:CLASS

```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 18:19:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     15 TO ITERATE

100.0% PROCESSED      15 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           68 TO      532
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 18:19:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    221 TO ITERATE

100.0% PROCESSED     221 ITERATIONS                               0 ANSWERS
SEARCH TIME: 00.00.01

L3             0 SEA SSS FUL L1
```

C:\Program Files\Stnexp\Queries\nucleo-260-E.str



chain nodes :
7 8 9 17 18 19 20 21 22 23 24 25 26 29 30 31 32 39 40 41 47 48 49 50
51 52 53 54 55 56 59 60 61
ring nodes :
1 2 3 4 5 6 12 13 14 15 16 33 34 35 36 37 38 42 43 44 45 46
chain bonds :
1-16 2-7 4-8 5-25 6-24 8-9 8-31 12-22 12-29 13-23 13-30 14-17 14-18 16-26
17-20 18-19 20-21 31-32 33-46 34-39 36-40 37-55 38-54 40-41 40-61 42-52 42-59
43-53 43-60 44-47 44-48 46-56 47-50 48-49 50-51
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-16 13-14 14-15 15-16 33-34 33-38 34-35 35-36
36-37 37-38 42-43 42-46 43-44 44-45 45-46
exact/norm bonds :
1-2 1-6 1-16 2-3 2-7 3-4 4-5 4-8 5-6 8-31 12-13 12-16 12-29 13-14 13-30
14-15 14-17 15-16 17-20 20-21 31-32 33-34 33-38 33-46 34-35 34-39 35-36 36-37
36-40 37-38 42-43 42-46 42-59 43-44 43-60 44-45 44-47 45-46 47-50 50-51
exact bonds :
5-25 6-24 8-9 12-22 13-23 14-18 16-26 18-19 37-55 38-54 40-41 40-61 42-52
43-53 44-48 46-56 48-49

G1:O,S,N,C

G2:H

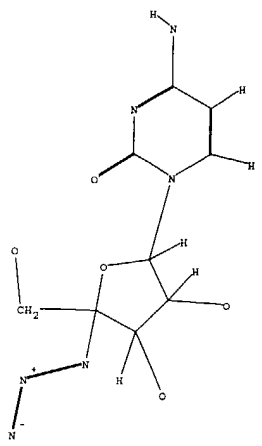
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:Atom
34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS 59:CLASS 60:CLASS 61:CLASS
fragments assigned product role:
containing 33
fragments assigned reactant/reagent role:

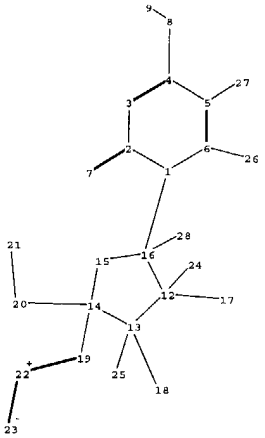
containing 1

```
=> s l4 sss sam
SAMPLE SEARCH INITIATED 18:34:29 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM      0 DOCUMENTS

100.0% DONE      0 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:         0 TO        0
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L4 (     0 REACTIONS)

=> s l4 sss full
FULL SEARCH INITIATED 18:34:37 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM      0 DOCUMENTS

100.0% DONE      0 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01

L6            0 SEA SSS FUL L4 (     0 REACTIONS)
```

```
=> d his

     (FILE 'HOME' ENTERED AT 18:30:03 ON 10 AUG 2004)

     FILE 'REGISTRY' ENTERED AT 18:30:17 ON 10 AUG 2004

     FILE 'CASREACT' ENTERED AT 18:30:22 ON 10 AUG 2004
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 SSS FULL
L4                STRUCTURE UPLOADED
L5              0 S L4 SSS SAM
L6              0 S L4 SSS FULL
```

C:\Program Files\Stnexp\Queries\nucleo-260-G.str





chain nodes :
7 8 9 17 18 19 20 21 22 23 24 25 26 27 28
ring nodes :
1 2 3 4 5 6 12 13 14 15 16
chain bonds :
1-16 2-7 4-8 5-27 6-26 8-9 12-17 12-24 13-18 13-25 14-19 14-20 16-28 19-22
20-21 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-16 13-14 14-15 15-16
exact/norm bonds :
1-2 1-6 1-16 2-3 2-7 3-4 4-5 4-8 5-6 12-13 12-16 12-17 13-14 13-18 14-15
14-19 15-16 19-22 22-23
exact bonds :
5-27 6-26 8-9 12-24 13-25 14-20 16-28 20-21

G1:O,S,N

G2:H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:Atom 13:Atom
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS